Current Status of NCSP Subtask 7 Subcritical Modeling

Kimberly Clark, D. Beller, A. Liu, L. Lakeotes University of Nevada Las Vegas





Statement of Work

- 1.1.1 Subcontractor shall assist Contractor in validating a developmental computational patch being added to the Los Alamos Monte Carlo N-Particle (MCNP) code's simulation capability for performing sub-critical neutron multiplication calculations through the following specific tasks:
 - Acquire and compile codes
 - MCNP5 v 1 51
 - MCNPX 2.6.0
 - MCNP-DSP
 - MCNP-PoliMi
 - PARTISN 5.97
 - Summarize relevant code capabilities
 - Perform simulations
 - Summarize simulation results and compare to MCNP5 multiplication (historic/ recent) results



Task 1 Status: Partially Completed

- All codes have been acquired
- MCNP5 v. 1.51, MCNPX 2.6.0, and MCNP-PoliMi have been successfully compiled
- MCNP-DSP has been compiled, however:
 - OS
 - Cross-section files
- PARTISN has been compiled
 - Cross-section sets have been compiled for use with code





Task 2 Status: Completed

- Relevant code capabilities beyond those of MCNP5 v. 1.51 have been summarized for:
 - MCNP-PoliMi
 - MCNP-DSP
 - PARTISN
- Limitations of MCNP5 v. 1.51:
 - User can define location, direction, energy, time, and intensity of SF and (α,n) neutron sources
 - User cannot define fission events
 - e.g. sample number of neutrons emitted from $v_{\sf bar}$
 - User **cannot** define correlated (time, location) neutron sources
 - MCNP samples these values from user's input
 - User <u>cannot</u> (easily) record location and time of detection.
 - Possible using MCNP's PTRAC capability and a user-created external script to extract this information
 - MCNPX some overlapping capability exists, but we are still investigating



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MCNP-PoliMi Overview

Modifications

- Analog particle tracking
- Correct neutron and gamma multiplicities have been included
- Correlation between neutron interaction and gamma production
- Conservation of energy for each interaction
- Secondary output file contains list mode data
 - Post-processing can be performed with included Matlab files to obtain detector response
 - Only for plastic scintillators
- Sources added
 - SF (Cf-252, U, Pu, Cm); Am-Be
 - Pu-Be and Am-Li to be added
- Can simulate up to 43 detector channels

Limitations

- No delayed neutrons
- No multigroup cross sections
- Limited to ENDF/B-VI and older



MCNP-PoliMi Overview

Sample output file:

| History number | Particle number | Projectile type I | nteraction type | Target nucleus | Cell number | Energy deposited (MeV) | Time (shakes) | Collisio | on position | (x, y ,z) | WGT | Generation number | Number of scatterings | Code |
|-------------------|--------------------|-------------------|-----------------|-------------------|----------------|---------------------------|------------------|----------|-------------|-----------|-----|----------------------|-----------------------|------|
| 16 | 97 | 1 | -99 | 1001 | 2 | 0.5309 | 8.095 | 43.57 | 4.88 | 1.84 | 1 | 3 | 5 | 0 |
| 16 | 97 | 1 | -99 | 1001 | 2 | 0.0553 | 8.395 | 44.29 | 5.57 | 1.85 | 1 | 3 | 6 | 0 |
| 16 | 97 | 1 | -99 | 1001 | 2 | 0.0014 | 11.722 | 44.92 | 5.04 | 3.78 | 1 | 3 | 9 | 0 |
| 109 | 1 | 1 | 0 | 6000 | 5 | 8.398 | 1.798 | 43.98 | -7.52 | 6.31 | 1 | 0 | 0 | 0 |
| 132 | 1 | 1 | -99 | 1001 | 5 | 13.9313 | 1.778 | 42.06 | -2.98 | 1.42 | 1 | 0 | 2 | 0 |
| 132 | 1 | 1 | -99 | 1001 | 5 | 0.1036 | 2.075 | 42.55 | -2.34 | 2.88 | 1 | 0 | 3 | 0 |
| 132 | 1 | 1 | -99 | 1001 | 5 | 0.0281 | 2.264 | 42.25 | -2.39 | 3.44 | 1 | 0 | 4 | 0 |
| 132 | 1 | 1 | -99 | 1001 | 5 | 0.0131 | 2.372 | 42.16 | -2.22 | 3.63 | 1 | 0 | 5 | 0 |
| 335 | 58 | 1 | -99 | 6000 | 4 | 0.0019 | 3.72 | 43.98 | 0.16 | 9.54 | 1 | 3 | 5 | 0 |
| 335 | 58 | 1 | -99 | 1001 | 3 | 0.0042 | 4.069 | 42.64 | -0.01 | 9.13 | 1 | 3 | 6 | 0 |
| 485 | 1 | 1 | -99 | 1001 | 5 | 8.2582 | 1.872 | 48.08 | -2.19 | 7.51 | 1 | 0 | 1 | 0 |
| 495 | 24 | 2 | 1 | 6 | 2 | 0.1461 | 1.036 | 43.87 | 3.46 | 5.06 | 1 | 1 | 2 | 0 |
| 495 | 24 | 2 | 1 | 6 | 2 | 1.2823 | 1.036 | 43.95 | 3.47 | 5.08 | 1 | 1 | 3 | -1 |
| 495 | 24 | 2 | 1 | 6 | 2 | 0.038 | 1.038 | 43.41 | 3.8 | 5.12 | 1 | 1 | 4 | -1 |
| 495 | 24 | 2 | 1 | 1 | 2 | 0.0793 | 1.038 | 43.28 | 3.76 | 5.08 | 1 | 1 | 5 | -1 |
| 495 | 24 | 2 | 1 | 6 | 2 | 0.0421 | 1.042 | 43.69 | 3.19 | 5.93 | 1 | 1 | 6 | -1 |

From S.A. Pozzi et al. / Nuclear Instruments and Methods in Physics Research A 513 (2003) 550–558



MCNP-DSP Overview

Modifications:

- Analog particle tracking
- Output given in data blocks of detector responses
- Correlates neutrons and gammas in time throughout fission chain mult. process
- Possible calculation modes: Source-driven noise analysis, Rossi-alpha, Pulsed source,
 Passive noise analysis, Multiplicity, Feynman variance
- Uses probability function P(v) rather than average v
- Angular distribution of prompt neutrons from fission
- Fission neutron energy distribution
- Prompt gamma ray mult. for SF isotopes and Cf-252; energy distribution for Cf-252
- Can simulate capture, scatter, and fission neutron and gamma detectors
- Can simulate detector dead time

Limitations:

- Based on outdated version of MCNP Format is not supported in Windows XP, Vista, 7
- Limited to ENDF/B-VI and older
- Limited to five detector channels



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PARTISN Overview

Modifications:

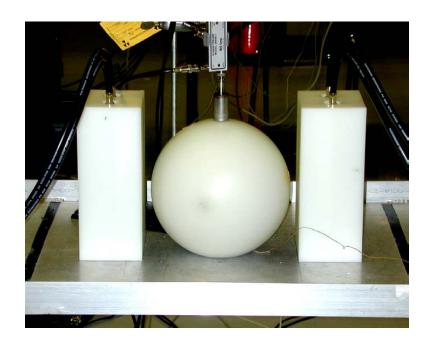
- Deterministic method numerically solves multigroup form of Boltzmann transport equation using discrete ordinates (Sn) method
- Modular structure separates input processing, transport equation solving, and postprocessing
- 1-D, 2-D, or 3-D geometries
- "diamond-differencing", adaptive weighted diamond differencing, and linear discontinuous or exponential discontinuous special differencing schemes
- Time-dependent calculations
- Deterministic Feynman-Y point model capability added recently (asymptotic and coincidence gate-width dependence)

Limitations:

- Multiplicative analysis capability being investigated
- Not as accurate as MC
 - Due to multi-group cross-sections, geometric representation



- Codes were compared using the BeRP Ball arrangement specified in the ICSBEP report SUB-PU-MET-FAST-001 in 3 configurations:
 - Bare
 - Surrounded by 3 inches of HDPE
 - Surrounded by 6 inches of HDPE (not done in benchmark)





- Kcode calculations have been completed with MCNP5 and MCNPX for the bare, 3-inch, and 6-inch arrangements
 - Results compared to benchmark to determine model validity
 - Calculations using both ENDF/B-VI and VII have been performed
- List mode data have been generated with MCNP-PoliMi for the bare and 3-inch arrangements
 - Feynman histograms will be created with post-processing code provided by LANL
- No results from MCNP-DSP or PARTISN at this time





Kcode calculation results:

| | Benchmark (MCNP/ENDF/B- VI) | MCNP5 1.51/ ENDF/B-VI | % difference | MCNPX 2.6.0/ ENDF/B-VI | % difference | |
|-----------|-----------------------------------|--------------------------|--------------|---------------------------|--------------|--|
| Bare | 0.77784±0.00004 | 0.77596±0.00006 | 0.24169 | 0.77563±0.00005 | 0.28412 | |
| 3-in Poly | 0.93721±0.00007 | 0.93693±0.00008 | 0.02988 | 0.93687±0.00009 | 0.03628 | |
| 6-in Poly | N/A | N/A | | N/A | | |

| | Benchmark (MCNP/ENDF/B- VI) | MCNP5 1.51/ ENDF/B-VII | % difference | MCNPX 2.6.0/ ENDF/B-VII | % difference | |
|-----------|-----------------------------------|---------------------------|--------------|----------------------------|--------------|--|
| Bare | 0.77784±0.00004 | 0.77762±0.00006 | 0.02828 | 0.77742±0.00005 | 0.05400 | |
| 3-in Poly | 0.93721±0.00007 | 0.93835±0.00008 | -0.12164 | 0.93835±0.00009 | -0.12164 | |
| 6-in Poly | N/A | N/A | | N/A | | |

Other calculations to perform:

- Neutron leakage tallies
- Detector efficiencies



MCNP-PoliMi output excerpt for 3-inch arrangement:

| particle number | | interaction type | target nucleus | cell number of collision event | energy deposited in collision (MeV) | time (shakes) | collision position (x, y, z) | | WGT | generation number | number of scatterings | code | |
|--------------------|---|---------------------|-------------------|--------------------------------|---|------------------|------------------------------|-------|------|----------------------|-----------------------|------|---|
| 18 | 1 | -99 | 2003 | 58 | 0.20624 | 1.019 | -26.28 | -2.29 | 1.84 | 1 | 0 | 1 | 0 |
| 12 | 1 | 0 | 2003 | 58 | 2.42073 | 1.026 | -24.51 | -2.54 | 6.18 | 1 | 0 | 1 | 0 |
| 15 | 1 | -99 | 2003 | 58 | 1.42718 | 1.053 | -25.15 | -3.17 | 2.34 | 1 | 0 | 1 | 0 |
| 11 | 1 | -99 | 2003 | 40 | 0.78974 | 1.169 | 25.25 | 2.97 | 5.92 | 1 | 0 | 1 | 0 |
| 9 | 1 | -99 | 2003 | 46 | 0.17272 | 1.347 | 25.11 | -2.11 | -0.4 | 1 | 0 | 2 | 0 |
| 6 | 1 | -99 | 2003 | 58 | 0.24532 | 1.386 | -25.13 | -3.12 | 3.31 | 1 | 0 | 2 | 0 |
| 10 | 1 | -99 | 2003 | 58 | 0.54088 | 1.739 | -25.97 | -3.35 | 3.84 | 1 | 0 | 3 | 0 |
| 11 | 1 | 0 | 2003 | 40 | 0.88908 | 2.357 | 25.15 | 2.62 | 6.67 | 1 | 0 | 2 | 0 |
| 6 | 1 | 0 | 2003 | 46 | 0.76822 | 2.448 | 24.46 | -2.39 | 3.08 | 1 | 0 | 3 | 0 |
| 14 | 1 | 0 | 2003 | 40 | 1.123 | 3.166 | 25.54 | 2.49 | 3.19 | 1 | 0 | 1 | 0 |
| 7 | 1 | -99 | 2003 | 58 | 0.13075 | 3.696 | -25.86 | -2.69 | 0.28 | 1 | 0 | 7 | 0 |
| 10 | 1 | 0 | 2003 | 52 | 0.79333 | 3.746 | -24.31 | 2.13 | 6.52 | 1 | 0 | 8 | 0 |
| 15 | 1 | 0 | 2003 | 40 | 0.7702 | 4.228 | 24.91 | 2.77 | 3.62 | 1 | 0 | 6 | 0 |
| 17 | 1 | 0 | 2003 | 40 | 0.78207 | 4.959 | 24.72 | 2.05 | 2.06 | 1 | 0 | 7 | 0 |
| 6 | 1 | 0 | 2003 | 46 | 0.76858 | 5.221 | 24.34 | -2.01 | 2.86 | 1 | 0 | 9 | 0 |
| 10 | 1 | 0 | 2003 | 52 | 0.77665 | 5.556 | -26.21 | 3.1 | 6.46 | 1 | 0 | 6 | 0 |
| 14 | 1 | 0 | 2003 | 46 | 0.76699 | 6.56 | 25.55 | -3.18 | 3.98 | 1 | 0 | 5 | 0 |
| 8 | 1 | 0 | 2003 | 58 | 0.76449 | 7.414 | -25.5 | -2.66 | 3.43 | 1 | 0 | 6 | 0 |
| 11 | 1 | 0 | 2003 | 40 | 0.76568 | 8.127 | 25.48 | 1.92 | 2.72 | 1 | 0 | 11 | 0 |



Task 4: Not Completed

- Report will be submitted upon completion of Tasks 1 through 3
 - Will contain the results of the simulations performed in Task 3 compared to the results from the simulations with the MCNP patch currently under development
 - Summaries of code capabilities will be included





Summary

- Quarterly reports have been submitted to LANL highlighting progress towards completion of tasks
 - Kcode simulations have been completed
 - List mode data
- Final report will be submitted upon completion comparing simulation results from the various codes with those from the patch



